

DOUGLAS JAY KLEIN – *Curriculum Vitae*

Professor Douglas Jay Klein was born on November 8, 1942 in Portland, Oregon. He got his B.Sc. degree in Chemistry at the Oregon State University, Corvallis in 1964. His postgraduate studies were completed at the University of Texas at Austin, where he got M.A. degree in Physical Chemistry in 1967 and Ph.D. in 1969. After obtaining the Ph.D. degree, he spent the next ten years at the University of Texas in Austin, the University of Cologne, Princeton University, and Rice University in Houston. In 1979, he joined Texas A&M University at Galveston (TAMUG) as an Assistant Professor, soon to be promoted to a position of Associate Professor and in 1987 he became Full Professor.

Professor Klein's research covers very diverse topics. Topics of his research interest are many, e.g., electronic structure of organic polymers, electron correlation in models for organic molecules, many-body valence-bond theory, chemical graph theory, theory of elemental carbon clusters, partial orderings in chemistry, theory of defects in extended structures, polymer statistics and excluded volume, group-theoretic methods in chemistry and physics, fractal structures in the natural sciences, anomalous diffusion, population dynamics models.

His research is supported by grants from the Welch Foundation in Houston. He has been an active member of the following societies: American Chemical Society, American Physical Society, Mathematical Association of America, American Mathematical Society and International Society for Mathematical Chemistry. Professor Klein is also Fellow of the International Academy of Mathematical Chemistry.

He was engaged as a referee for a number of journals, e.g. *Croatica Chemica Acta*, *Journal of Mathematical Chemistry*, *International Journal of Quantum Chemistry*, *Journal of Chemical Information and Computer Science*, *MATCH Communications in*

Mathematical and in Computer Chemistry, *Physical Review B*, *Journal of the American Chemical Society*, *Theoretica Chimica Acta*, *Journal of the Chemical Society*, *Journal of Physics A*, *Journal of Chemical Education*, *Physical Review Letters*, *Discrete Applied Mathematics*, *Chemical Physics Letters*, *Journal of Chemical Physics*. He was also reviewer for some granting agencies, including NSF.

Professor Klein also edited two books: D. J. Klein and N. Trinajstić, *Valence-Bond Theory and Chemical Structure* (Elsevier, Amsterdam, 1990) and D. J. Klein and M. Randić, *Mathematical Chemistry* (VCH Pub., New York, 1990).

He also edited special issues of the following journals: D. J. Klein and M. Randić, *Journal of Mathematical Chemistry* 7 (1990) dedicated to the 3rd International conference on Mathematical Chemistry, D. J. Klein and J. Brickmann, special issue of *MATCH Communications in Mathematical Chemistry and in Computer Chemistry* vol. 42 (2000) dedicated to applications of partial orderings in chemistry and D. J. Klein, special issue of *Internet Electronic Journal of Molecular Design*, vol. 11 (2003) dedicated to Professor Nenad Trinajstić.

He was given the TAMU distinguished achievements award in research (1992), and Fulbright Fellowship at Oxford (1994).

Professor Klein was a member of the following Editorial Advisory Boards: *Journal of Mathematical Chemistry* (1988–2006), *MATCH Communications in Mathematical and in Computer Chemistry* (1994–), *International Journal of Quantum Chemistry* (1990–1993), *Fullerene Science & Technology* (1994–2003) and *Croatica Chemica Acta* (1995–).

Nenad Trinajstić

DOUGLAS JAY KLEIN – *List of Publications*

Scientific Articles

1. D. J. Klein, E. M. Greenawalt & F. A. Matsen, "The adjustment of Ab Initio Potential Curves", *Journal of Chemical Physics* **47** (1967) 4820–4823.
2. D. J. Klein, C. E. Rodriguez, J. C. Browne & F. A. Matsen, "The Ground-State of He₂", *Journal of Chemical Physics* **47** (1967) 4862–4863.
3. F. A. Matsen & D. J. Klein, "Spin-Free Quantum Chemistry. VI. Spin Conservation", *Journal of Physical Chemistry* **73** (1969) 2477–2487.
4. D. J. Klein, "Local Permutational Symmetry and the Separated Atom Limit", *Journal of Chemical Physics* **50** (1969) 5140–5150.
5. D. J. Klein, "The Interaction of Two Metastable Triplet Helium Atoms", *Journal of Chemical Physics* **50** (1969) 5151–5157.
6. F. A. Matsen & D. J. Klein, "Spin Conservation", pages 1–55 in *Advances in Photochemistry*, Vol. VII, ed. by W. A. Noyes, Jr., G. S. Hammond and J. N. Pitts, Jr., (John Wiley and Sons, 1969).
7. D. J. Klein & R. W. Kramling, "The Symmetry of Reduced Density Matrices. I. General Algebraic Formulation", *International Journal of Quantum Chemistry* **S 4** (1970) 661–674.
8. D. J. Klein, "The Symmetry of Reduced Density Matrices. II. Spin-Free Quantum Chemistry and Point Group Symmetry", *International Journal of Quantum Chemistry* **S 3** (1970) 675–688.
9. D. J. Klein, C. H. Carlisle & F. A. Matsen, "Symmetry Adaptation to Sequences of Finite Groups", pages 219–260 in *Advances in Quantum Chemistry*, Vol. 5, ed. P. O. Lowdin (Academic Press, 1970).
10. D. J. Klein, "Symmetry Adapted Perturbation Theory for Interatomic and Intermolecular Exchange Energies", *International Journal of Quantum Chemistry* **S 4** (1971) 271–283.
11. D. J. Klein, R. D. Poshusta, B. R. Junker & F. A. Matsen, "Computation in the Spin-Free Formulation of the Polyelectronic Problem", *International Journal of Quantum Chemistry* **S 4** (1971) 141–146.
12. D. J. Klein & B. R. Junker, "Spin-Free Computation of Matrix Elements I: Group Theoretical Computation of Pauling Numbers", *Journal of Chemical Physics* **54** (1971) 4290–4296.
13. D. J. Klein & Z. G. Soos, "Site Representation for Charge Transfer Excitations in Molecular Crystals", *Molecular Physics* **20** (1971) 1013–1024.
14. D. J. Klein, "Variational Scheme for Multistate Kets", *Physical Review A* **3** (1971) 528–532.
15. F. A. Matsen & D. J. Klein, "Spin-Free Quantum Chemistry. IX. The Aggregate Theory of Polyelectronic Systems", *Journal of Physical Chemistry* **75** (1971) 1860–1865.
16. F. A. Matsen, D. J. Klein & D. C. Foyt, "Spin-Free Quantum Chemistry. X. The effective Spin Hamiltonian", *Journal of Physical Chemistry* **75** (1971) 1866–1873.
17. Z. G. Soos & D. J. Klein, "Modified Hubbard Model for Complex TCNQ Salts", *Journal of Chemical Physics* **55** (1971) 3284–3290.
18. B. R. Junker & D. J. Klein, "Spin-Free Computation of Matrix Elements II: Simplifications Due to Invariance Groups", *Journal of Chemical Physics* **55** (1971) 5532–5542.
19. D. J. Klein, D. Hankins, and R. W. Kramling, "Simple Construction of Point Group Degenerate Wave Functions", *International Journal of Quantum Chemistry* **6** (1972) 1101–1117.
20. W. A. Seitz & D. J. Klein, "Computations on Heisenberg Spin Models", *International Journal of Quantum Chemistry* **7** (1973) 647–665.
21. D. J. Klein, "A Group-Theoretic View of Weakly Interacting Sites", pages 193–207 in *Wave Mechanics – The First Fifty Years*, ed. W. C. Price, S. S. Chissick and T. Ravendale (Butterworth and Co., London, 1973).
22. D. J. Klein & W. A. Seitz, "Perturbation Expansion of the Linear Hubbard Model", *Physical Review B* **8** (1973) 2236–2247.
23. D. C. Foyt & D. J. Klein, "Multistate Kets for the Hydrogen Molecule", *Physical Review A* **8** (1973) 2274–2279.
24. D. J. Klein & D. C. Foyt, "Variational Multistate Ket Derivation of the Heisenberg Spin Hamiltonian", *Physical Review A* **8** (1973) 2280–2287.
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29. W. A. Seitz & D. J. Klein, "Static Thermodynamic Properties of the Linear Half-filled Hubbard Model", *Physical Review B* **9** (1974) 2159–2164.
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34. Z. G. Soos & D. J. Klein, "Charge-Transfer in Solid State Complexes", pages 1–109 in *Molecular Associations*, Vol. I, (Academic Press, New York, 1975).
35. A. A. Cantu, D. J. Klein, F. A. Matsen & T. H. Seligman, "A Second-Quantized Formulation of Valence-Bond Theory", *Theoretica Chimica Acta* **38** (1975) 341–354.
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39. D. J. Klein, "Variational Localized-Site Cluster Expansions. III. Point Group Symmetry and Supersymmetry", *Molecular Physics* **31** (1976) 783–796.
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